Building a PDE Code from Components, Including

Shape Optimization and Embedded UQ

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Introduction

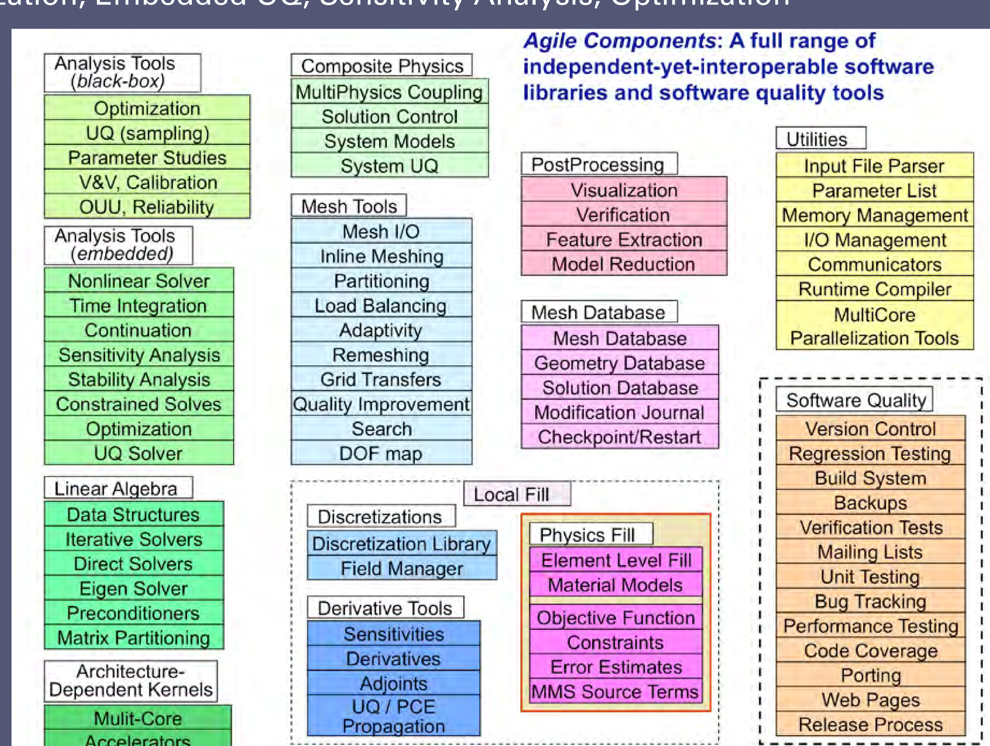
Agile Components is a strategic effort at Sandia to maximize our impact as computational scientists. The central idea is for all projects to both leverage and contribute to a common base of knowledge and software. This builds the foundation for impacting future projects.

Agile Components implementation plan:

- Develop a full range of independent yet interoperable software components, both: ☐Capabilities ☐Interfaces
- Adopt high standards for Software Quality tools and procedures
- Develop prototype applications that mature and demonstrate capabilities and interoperability, and drive development

Agile Components stretch goals:
Rapid development of PDE codes for new applications
- New codes can developed in 2 FTEs

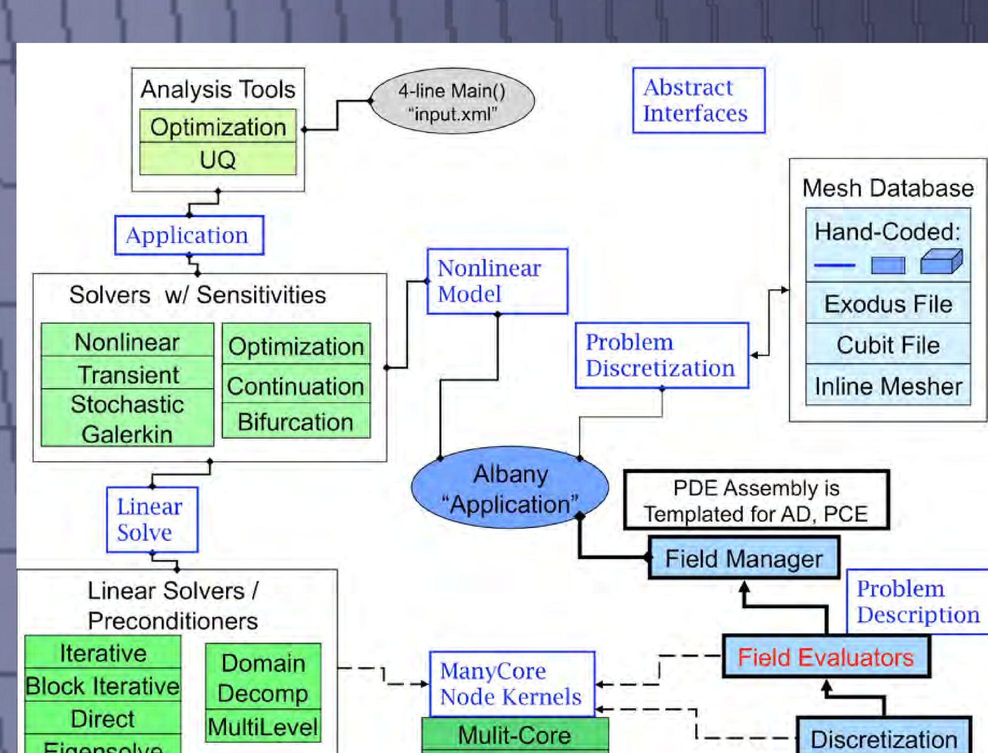
PDE code born with transformational analysis capabilities
- Shape Optimization, Embedded UQ, Sensitivity Analysis, Optimization



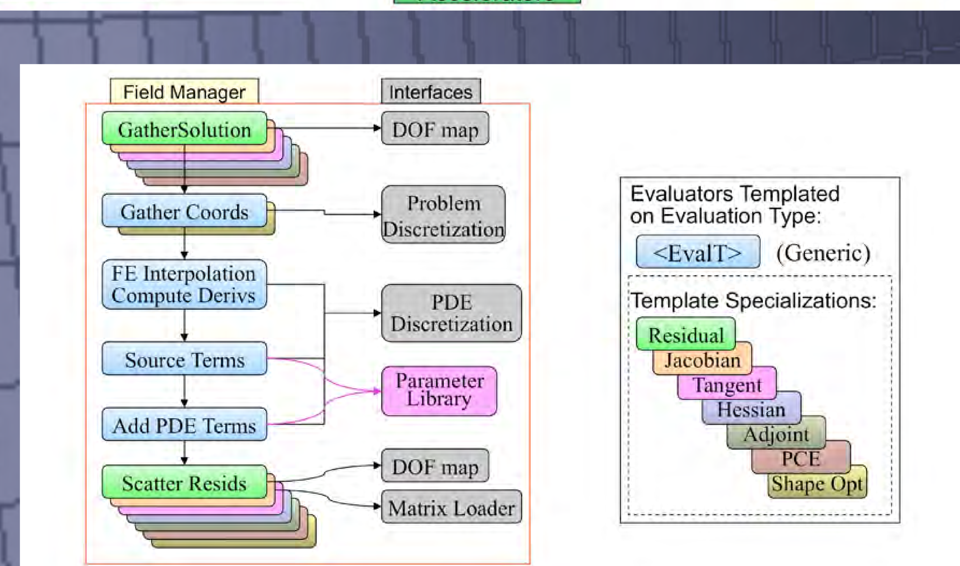
Part II

Albany is an Agile Components demonstration application that has been used to drive development of the vision, and measure progress towards the stretch goals. Albany has interfaces to most of the algorithms delivered through Trilinos, Dakota, Cubit, and Sierra Toolkit libraries. The code design differs from a monolithic framework in that well-defined abstract interfaces keep a clear separation of concerns.

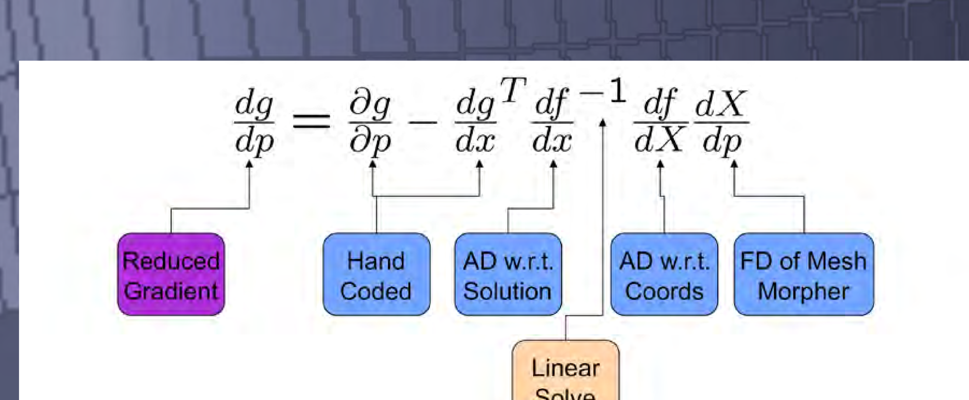
Software Design of Albany, an Open Source Agile Components demonstration code:



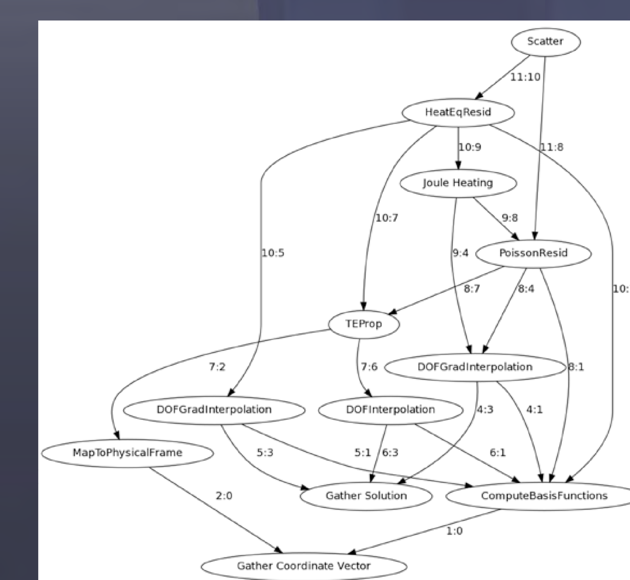
The stretch goals of (A) the rapid development of new PDE applications and (B) the embedding of transformational analysis algorithms are reachable in large part by the use of templated field evaluators. When data types for Automatic Differentiation and Polynomial Chaos Expansions are appropriately seeded, and passed through the PDE residual evaluation, analytic Jacobians, Tangents, and Stochastic Expansions are automatically generated.



Shape optimization is a special case where derivatives with respect to the coordinate vector X are required. The reduced gradient which is needed for gradient-based optimization algorithms, is assembled using a variety of differentiation methods.



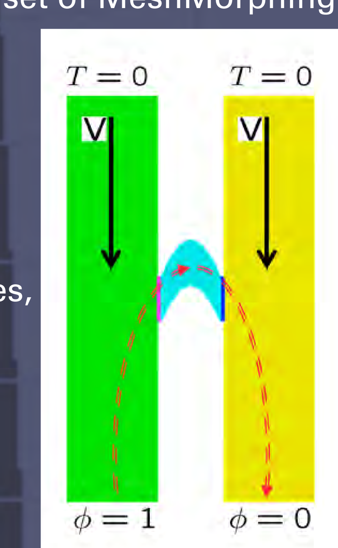
Field Manager with Field Evaluators For Sliding ElectroMagnetic Contact Application



Part III

Sliding ElectroMagnetic Contact Demonstration: In this application, a slider (blue) is propelled between two conductors (green and yellow) when a current is passed through it (red dashed line). The design optimization problem is to find the shape of the slider that minimizes the temperature increase.

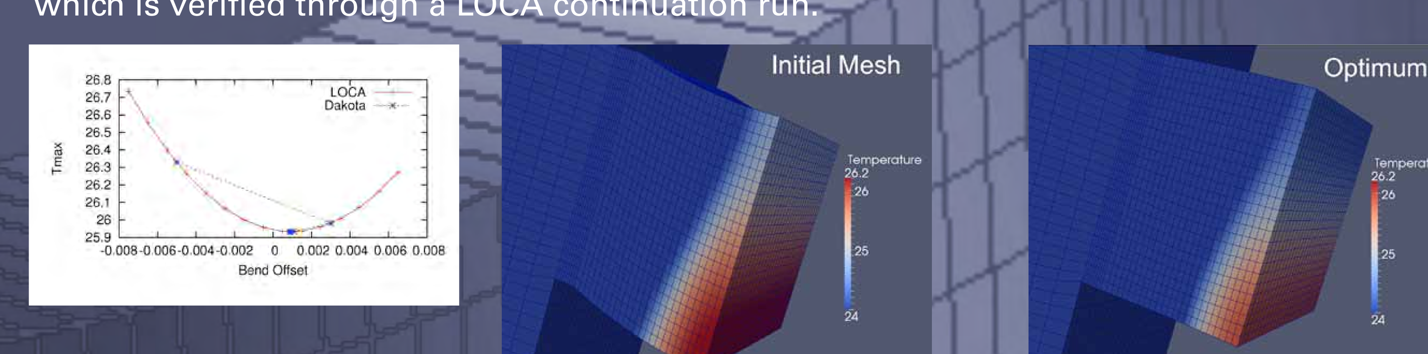
The shape is parameterized by 3 parabolas in the Cubit mesh generator. A set of MeshMorphing algorithms are under development, which reprocess the coordinate positions as a function of geometry changes.



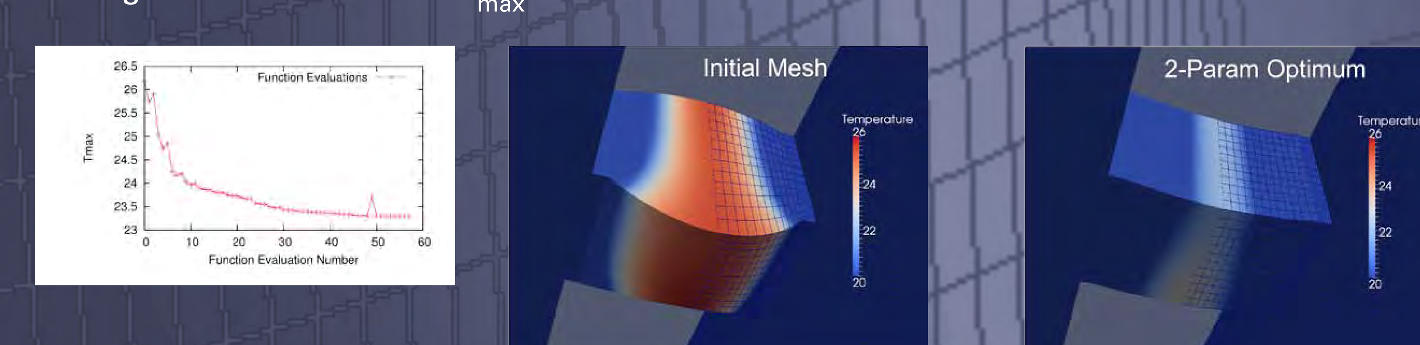
The current is simulated by a potential equation with a proscribed voltage drop. The heat equation captures conduction, convection, and a nonlinear joule heating term. Since the electrical permittivity is inversely dependent on the temperature, the two PDEs are coupled and nonlinear. The properties, such as σ_0, vary by material. A quasi-steady approximation is used.

$$\begin{aligned} -\nabla \cdot \sigma \nabla \phi &= 0 \\ -\nabla \cdot \kappa \nabla T - \mathrm{v} \cdot \nabla T &= \sigma (\nabla \phi)^2 \\ \sigma(T) &= \sigma_0 / [1 + \beta (T - T_0)] \end{aligned}$$

A 1-parameter design problem is solved with a gradient-based optimization algorithm in Dakota, which is verified through a LOCA continuation run.



Three parabolic deflections (leading edge, trailing edge, and z-bulge), when subject to a volume constraint on the slider, result in a 2-parameter design optimization. The optimization run results in a significant decrease of T_{max}



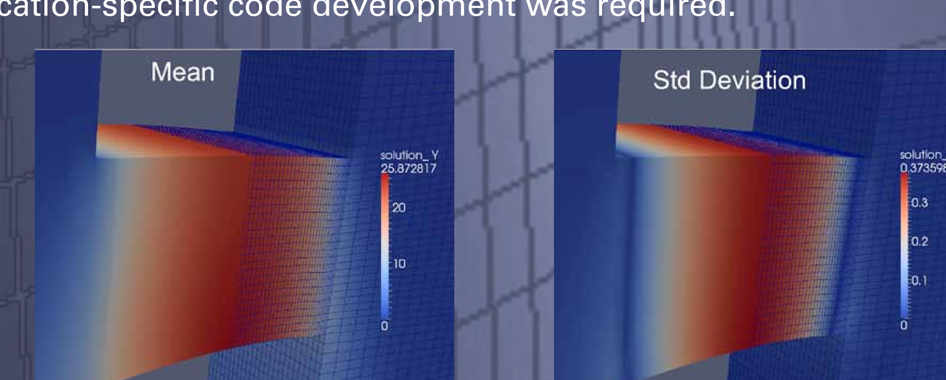
Embedded UQ capability: A UQ Study was performed for the 3D model. PCE expansions are automatically propagated through the PDEs. The full stochastic nonlinear system is solved with Newton's Methods. No application-specific code development was required.

The base electrical conductivity in the thin gap regions is gien the following distribution:

$$\sigma_0^g = 35.0 P_0(\xi) + 15.0 P_1(\xi)$$

leading to a polynomial expansion in Tmax

$$T_{Max} = 25.87 P_0(\xi) + 0.61 P_1(\xi) - 0.17 P_2(\xi) + 0.04 P_3(\xi)$$



Conclusions: The Agile Components strategy is to assemble a comprehensive set of independent-yet-interoperable software libraries, abstract interfaces, and software quality procedures. With this infrastructure and knowledge base, new PDE codes can be rapidly written from scratch. By writing a templated PDE assembly, one can just write the residual equations and a whole host of information is generated automatically. This provides the quantities needed for transformational analysis algorithms.

As a demonstration, we created a simulator for a 3D coupled nonlinear model: sliding electromagnetic contact. With just adding a few evaluators for the PDE terms, all the infrastructure was in place to perform Shape Optimization and embedded UQ.

Acknowledgements: The Agile Components strategy relies on the collected efforts of the Trilinos, Dakota, Sierra Toolkit, and Cubit teams. We'd like to thank the developers, managers, and funding sources for these assemblies of projects. In particular, the ASC and ASCR programs at DOE.

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